



## Lithium Dinitramide as an Additive in Lithium Power Cells

**This inorganic additive appears to act as a superior SEI promoter.**

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Lithium dinitramide,  $\text{LiN}(\text{NO}_2)_2$  has shown promise as an additive to non-aqueous electrolytes in rechargeable and non-rechargeable lithium-ion-based electrochemical power cells. Such non-aqueous electrolytes consist of lithium salts dissolved in mixtures of organic ethers, esters, carbonates, or acetals. The benefits of adding lithium dinitramide (which is also a lithium salt) include lower irreversible loss of capacity on the first charge/discharge cycle, higher cycle life, lower self-discharge, greater flexibility in selection of electrolyte solvents, and greater charge capacity.

The need for a suitable electrolyte additive arises as follows: The metallic lithium in the anode of a lithium-ion-based power cell is so highly reactive that in addition to the desired main electrochemical reaction, it engages in side reactions that cause formation of resistive films and dendrites, which degrade performance as quantified in terms of charge capacity, cycle life, shelf life, first-cycle irreversible

capacity loss, specific power, and specific energy. The incidence of side reactions can be reduced through the formation of a solid-electrolyte interface (SEI) — a thin film that prevents direct contact between the lithium anode material and the electrolyte. Ideally, an SEI should chemically protect the anode and the electrolyte from each other while exhibiting high conductivity for lithium ions and little or no conductivity for electrons. A suitable additive can act as an SEI promoter.

Heretofore, most SEI promotion was thought to derive from organic molecules in electrolyte solutions. In contrast, lithium dinitramide is inorganic. Dinitramide compounds are known as oxidizers in rocket-fuel chemistry and until now, were not known as SEI promoters in battery chemistry. Although the exact reason for the improvement afforded by the addition of lithium dinitramide is not clear, it has been hypothesized that lithium dinitramide competes with other electrolyte constituents

to react with lithium on the surface of the anode to form a beneficial SEI. Apparently, nitrides and oxides that result from reduction of lithium dinitramide on the anode produce a thin, robust SEI different from the SEIs formed from organic SEI promoters. The SEI formed from lithium dinitramide is more electronically insulating than is the film formed in the presence of an otherwise identical electrolyte that does not include lithium dinitramide. SEI promotion with lithium dinitramide is useful in batteries with metallic lithium and lithium alloy anodes.

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*Inquiries concerning rights for the commercial use of this invention should be addressed to NASA Glenn Research Center, Innovative Partnerships Office, Attn: Steve Fedor, Mail Stop 4-8, 21000 Brookpark Road, Cleveland, Ohio 44135. Refer to LEW-17983-1.*



## Accounting for Uncertainties in Strengths of SiC MEMS Parts

**Fracture strength of a part can be predicted as one statistical distribution.**

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A methodology has been devised for accounting for uncertainties in the strengths of silicon carbide structural components of microelectromechanical systems (MEMS). The methodology enables prediction of the probabilistic strengths of complexly shaped MEMS parts using data from tests of simple specimens. This methodology is intended to serve as a part of a rational basis for designing SiC MEMS, supplementing methodologies that have been borrowed from the art of designing macroscopic brittle material structures.

The need for this or a similar methodology arises as a consequence of the fundamental nature of MEMS and the brittle silicon-based materials of which they are typically fabricated. When tested to fracture, MEMS and structural components

thereof show wide part-to-part scatter in strength. The methodology involves the use of the Ceramics Analysis and Reliability Evaluation of Structures Life (CARES/Life) software in conjunction with the ANSYS Probabilistic Design System (PDS) software to simulate or predict the strength responses of brittle material components while simultaneously accounting for the effects of variability of geometrical features on the strength responses. As such, the methodology involves the use of an extended version of the ANSYS/CARES/PDS software system described in "Probabilistic Prediction of Lifetimes of Ceramic Parts" (LEW-17682-1/4-1), *Software Tech Briefs* supplement to *NASA Tech Briefs*, Vol. 30, No. 9 (September 2006), page 10.

The ANSYS PDS software enables the ANSYS finite-element-analysis program to account for uncertainty in the design-and-analysis process. The ANSYS PDS software accounts for uncertainty in material properties, dimensions, and loading by assigning probabilistic distributions to user-specified model parameters and performing simulations using various sampling techniques. The CARES/Life code predicts the time-dependent probabilities of failure of brittle material structures under thermomechanical loads.

In the present methodology, CARES/Life is used with ANSYS/PDS to simulate the effect of variations of dimensions on the predicted probabilities of failure of SiC specimens. A special ANSYS macroinstruction code was developed for this pur-